The Phase Structure of Grain Boundaries

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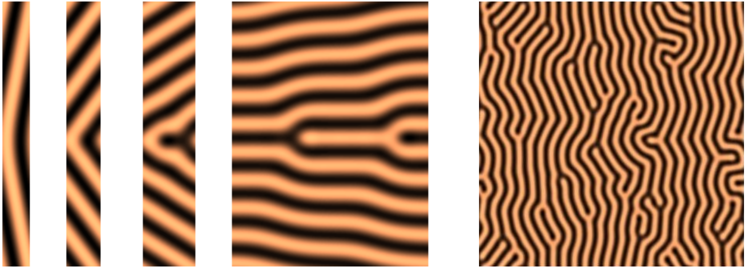


Joint work with Nick Ercolani & Nikola Kamburov

Outline

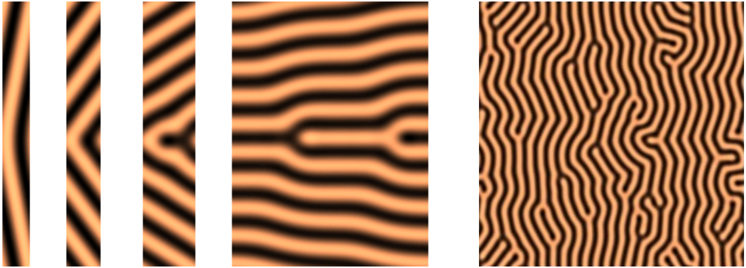
1. Grain boundaries of the Swift-Hohenberg equation (SH)
    - The Swift-Hohenberg equation: roll patterns and grain boundaries
    - Numerical simulations
    - The phase structure of grain boundaries
2. Grain boundaries of the Regularized Cross-Newell Equation
    - Self-dual "knee" solutions
    - When phase gradients are not constrained be vector fields
3. Grain boundary solutions of the Swift-Hohenberg Equation revisited
4. Summary and open questions

Grain boundaries of the Swift-Hohenberg equation

$$\frac{\partial \psi}{\partial t} = R\psi - (1 + \nabla^2)^2 \psi - \psi^3$$

- The Swift-Hohenberg (SH) equation is a canonical pattern-forming model.
- It admits a family of roll pattern solutions.
- We are interested in a particular class of defects, grain boundaries, which separate regions of roll patterns with different orientation.

Grain boundaries of the Swift-Hohenberg equation



- Existence near threshold for translation-invariant cores was proved for all angles between roll patterns.
- A full numerical study of grain boundaries, including those without translation-invariant cores, was recently performed.

Grain boundaries of the Swift-Hohenberg equation

It has been known for many years that grain boundaries of the SH equation undergo a core instability when the angle α exceeds a critical value (or when k_y is smaller than some threshold value).

Right: Numerical simulations of SH with $R = 1$.

N. Ercolani, R. Indik, A.C. Newell, & T. Passot, *Global Description of Patterns Far From Onset: A Case Study*, Physica **D 184**, 127-140 (2003).

Grain boundaries of the Swift-Hohenberg equation

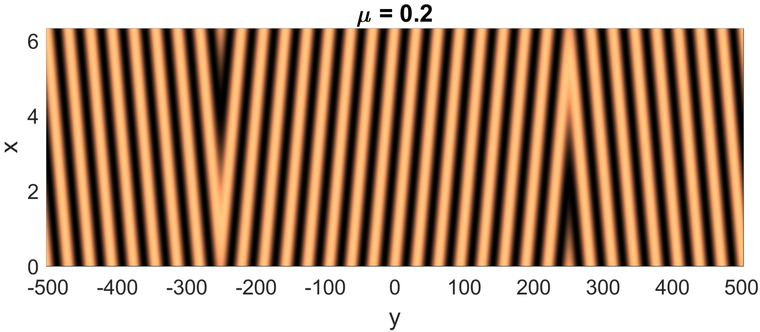
This instability provides a paradigm to understand the connection between defects and phase.

- To this end, we turn to numerical simulations of the Swift-Hohenberg equation.
- The use of a pseudo-spectral code with periodic boundary conditions makes it easy to find the amplitude of each pattern on each side of the grain boundary.
- One can then view each grain boundary as a heteroclinic connection between the two asymptotic patterns, thereby setting the stage for a description in terms of spatial dynamics.
- It is also possible to estimate the phase of the solution and therefore connect to the phase diffusion equation.

Numerical simulations of SH grain boundaries

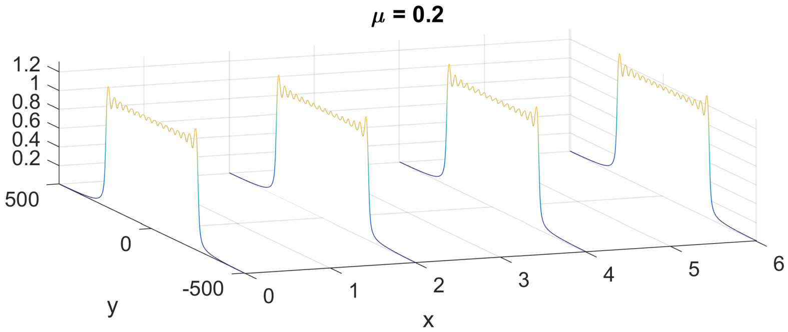
- The simulation box has size $L_x = 2\pi/k_1$, where $k_1 = \sqrt{1-\mu^2}$, $0 < \mu < 1$, and $L_y \simeq 1000$.
- The initial conditions consist of two regions of rolls of wavevector $\vec{k}_+ = (k_1, \mu)$ and $\vec{k}_- = (k_1, -\mu)$, separated by two straight lines parallel to the x-axis.
- Long-time solutions of the simulation are (for all practical purposes) stationary.

Grain boundaries of the Swift-Hohenberg equation



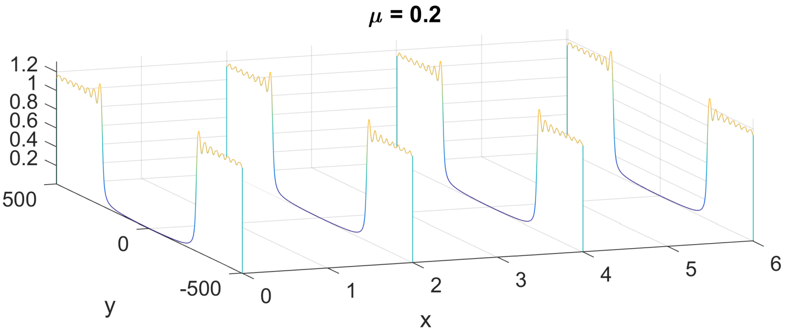
Pattern for $\mu = 0.2$ as a function of x and y

Grain boundaries of the Swift-Hohenberg equation



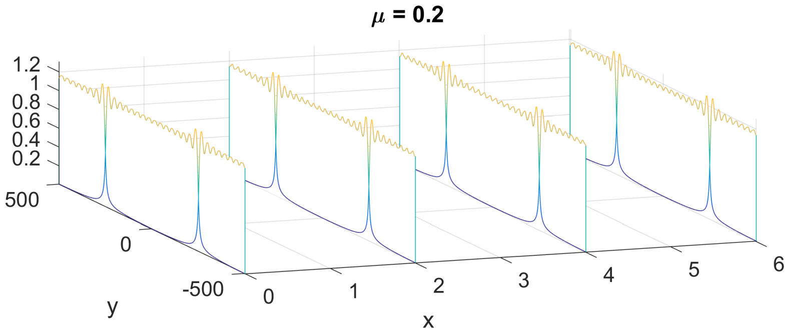
Envelope of 'zig' pattern as a function of x and y

Grain boundaries of the Swift-Hohenberg equation



Envelope of 'zag' pattern as a function of x and y

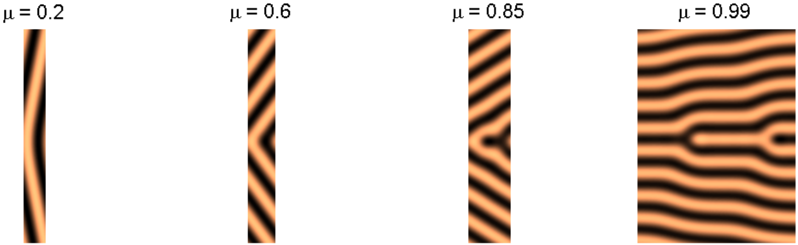
Grain boundaries of the Swift-Hohenberg equation



Envelope of both patterns as a function of x and y, showing two heteroclinic orbits corresponding to two grain boundaries

Numerical simulations of SH grain boundaries

As the parameter μ increases, two dislocations appear per period at the core of the grain boundary.

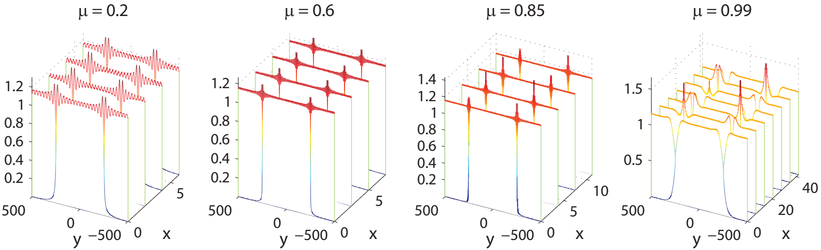


Solutions at $t = 20,000$ (left two panels) and $t = 10,000$ (right 2 panels). The vertical extent of each picture corresponds to 60 units of length (recall $L_y \simeq 1000$).

Similar results were recently obtained in D.J.B. Lloyd & A. Scheel, *Continuation and Bifurcation of Grain Boundaries in the Swift-Hohenberg Equation*, SIAM J. Appl. Dyn. Sys. **16**, 252-293 (2017).

Numerical simulations of SH grain boundaries

Our numerical investigations suggest that the appearance of dislocations in a grain boundary is linked to a symmetry breaking bifurcation that alters translational invariance along its core.



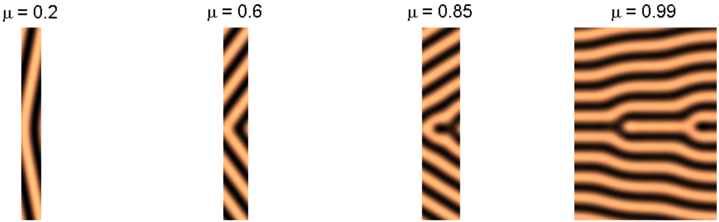
Solutions at $t = 20,000$ (left two panels) and $t = 10,000$ (right 2 panels).

As μ increases, the profiles lose translational invariance along the x-direction.

The phase structure of grain boundaries

- These simulations may be used to document changes in the phase structure of grain boundaries as the angle of inclination of the rolls is varied.
- Taking the Hilbert transform of a grain boundary solution u of SH in a direction parallel to its core, leads to a complex field z such that $\Re(z) = u$.
- We define the phase θ of the solution by $z = |z| \exp(i\theta)$.
- For small values of μ, the component k_y of $\vec{k} = \nabla\theta$ perpendicular to the grain boundary changes direction by vanishing at the core of the defect.

The phase structure of grain boundaries



- As μ increases, k_y develops a "jump" on each side of the grain boundary.
- The x-dependence of the phase θ along the "jump" shows
  - regions where θ is constant,
  - alternating with regions where θ is linear and θ_y is constant.

Together, these suggest mixed boundary conditions for the phase at the core of a grain boundary.

The phase structure of grain boundaries

- Hopefully by now I have convinced you that these dislocations are related to changes in the phase structure of the pattern.
  - When dislocations are present, maxima of θ_y "jump" across the core of the grain boundary.
  - The boundary conditions on each side of the core are mixed: regions of constant θ alternate with regions where θ_y is constant.
- So it is natural to ask whether one sees similar behaviors in the corresponding phase diffusion equation, which is what we will now turn to.
- Far from threshold, the phase of SH roll solutions is formally described by the Regularized Cross-Newell equation (RCN).

Grain boundary solutions of the phase diffusion equation

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \left(2\vec{k}(1-k^2) + \Delta \vec{k} \right), \qquad \vec{k} = \nabla \theta \qquad \text{(RCN)}$$

- Far from threshold, i.e. for $R = O(1)$, roll patterns are well described by the regularized Cross-Newell equation (RCN).
- Since RCN is variational, it is reasonable to ask whether the the birth of defects at the core of grain boundaries may be understood by analysing minimizers of the RCN energy as μ is increased.
- Grain boundaries of the SH equation correspond to exact self-dual ("knee") solutions of RCN.

Grain boundary solutions of the phase diffusion equation

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \left(2\vec{k}(1-k^2) + \Delta \vec{k} \right), \qquad \vec{k} = \nabla \theta \qquad \text{(RCN)}$$

- Self-dual solutions of RCN are such that $\Delta\theta = \pm(1 - |\nabla\theta|^2)$.

$$\mathcal{E}_{RCN} = \int_\Omega \left[(\Delta\theta)^2 + (1 - |\nabla\theta|^2)^2 \right] \, d\Omega$$

  They can be expressed in terms of their boundary data, $\theta_y(x)$, at the core of the grain boundary.

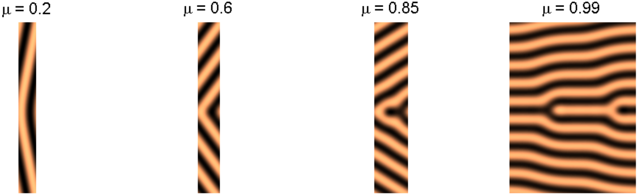
- We can prove that self-dual knee solutions of RCN are minimizers of the RCN energy, regardless of the value of μ, if we demand that phase gradients be vector fields.

Grain boundary solutions of the phase diffusion equation

$$\frac{\partial\theta}{\partial t} = -\nabla\cdot\left(2\vec{k}(1-k^2)+\Delta\vec{k}\right), \qquad \vec{k} = \nabla\theta \qquad \text{(RCN)}$$

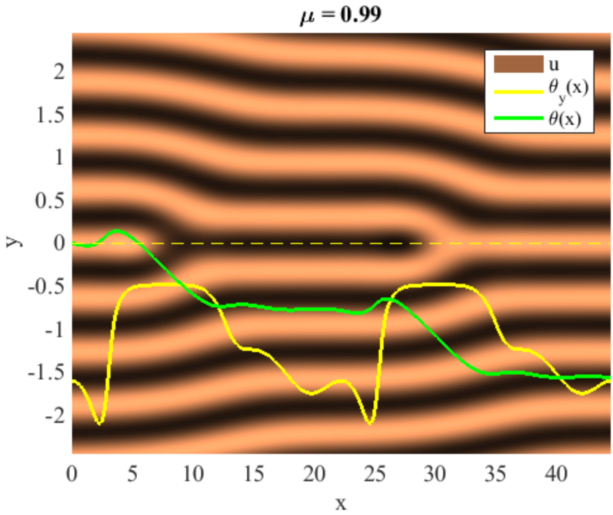
- It is however known that if this requirement is relaxed, there exist solutions of lower energy as μ is increased.
- In that case, RCN solutions resembling bifurcated grain boundaries were numerically obtained by imposing mixed boundary conditions at the core of the defect.
- These solutions are expected to only deviate from self-duality near the core of each dislocation.

Grain boundary solutions of SH revisited



- For small values of μ, grain boundary solutions of SH have a phase that behaves like self-dual solutions of RCN.
- As μ increases, the phase moves away from self-duality near the core of the grain boundary.
- At the same time, it develops large y-derivatives that "jump" across the grain boundary, with regions of constant phase θ alternating with regions of constant θ_y along the jump.

Phase structure of SH Grain boundaries



Profile of θ and θ_y on one side of the "jump" as a function of x superimposed on the grain boundary solution.

Summary and open questions

- There is ample numerical evidence that large phase derivatives lead to defect formation.

- The mixed boundary conditions found from the numerical simulations of SH are slightly different from those used to find minimizing solutions of RCN.

  $\rightarrow$ Does this suggest solutions of RCN that have lower energy than the solutions found so far?

- Solutions of SH are smooth and the phase extracted from these solutions is regular at the core of the grain boundary.

  $\rightarrow$ Is it legitimate to assume that solutions of RCN represent the "large scale" behavior of the phase of SH solutions?

- If so, it may be possible to bridge the gap between RCN and SH grain boundaries.

Roadmap

- Analyze the stability of grain boundaries in SH near and far from threshold.
  - In particular, "knee" solutions of SH should become unstable as μ gets close to 1.
- Identify candidate minimizers of RCN
  - Use the boundary data suggested by SH simulations to define self-dual solutions of RCN, and estimate their energy.
  - Alternatively, seek non self-dual solutions of RCN that closely approximate these new numerical solutions.
  - The level of regularity of RCN grain boundaries would describe how a pattern-forming system leaves its phase approximation.

The Swift-Hohenberg equation

- The Swift-Hohenberg (SH) equation

$$\frac{\partial \psi}{\partial t} = R\psi - (1 + \nabla^2)^2 \psi - \psi^3$$

is a canonical pattern-forming model.

- It is variational

$$\frac{\partial \psi}{\partial t} = -\frac{\delta \mathcal{E}_{SH}}{\delta \psi} \qquad \text{where} \qquad \mathcal{E}_{SH} = \int_{\Omega} e_{SH} \; d\Omega$$

and

$$e_{SH} = -\frac{R}{2}\psi^2 + \frac{1}{2}\left((1 + \nabla^2)\psi\right)^2 + \frac{\psi^4}{4}.$$

J. Swift & P.C. Hohenberg, *Hydrodynamic fluctuations at the convective instability*, Phys. Rev. **A 15**, 319-328 (1977).

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Roll solutions of the Swift-Hohenberg equation

For $R > 0$ small and $|k| \gtrsim 1$, the SH equation possesses a stable family of stationary roll solutions of the form

$$\begin{aligned} \psi_0(x,y) &= \psi_0(\theta) \\ &= a_1(k)\cos(\theta(x,y)) + \mathcal{O}(\epsilon^{3/2}), \\ \theta(x,y) &= k\cos(\alpha)\,x + k\sin(\alpha)\,y, \quad \alpha \in \mathbb{R} \end{aligned}$$

with $\epsilon = |R - (k^2-1)^2|$.

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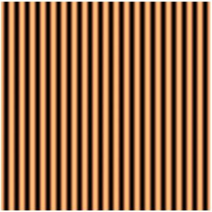

- A. Mielke, *A new approach to sideband-instabilities using the principle of reduced instability*, in Nonlinear Dynamics and Pattern Formation in the Natural Environment (eds.: A. Doelman, A. van Harten) Longman UK, 206-222 (1995).

- G. Schneider, *Diffusive Stability of Spatial Periodic Solutions of the Swift-Hohenberg Equation*, Comm. Math. Phys. **178**, 679-702 (1996).

- A. Mielke, *Instability and stability of rolls in the Swift-Hohenberg equation*, Comm. Math. Phys. **189**, 829-853 (1997).

- H. Uecker, *Diffusive stability of rolls in the two-dimensional real and complex Swift-Hohenberg equation*, Comm. PDE **24**, 2109-2146 (1999).

Grain boundaries of the Swift-Hohenberg equation

- For $R > 0$ small enough, the SH equation possesses a family of grain boundary solutions in the form of one-dimensional heteroclinic orbits. These solutions have envelopes that are translationally invariant along the core of the grain boundary.
- They connect roll patterns with asymptotic phases of the form $\theta_1(x, y)$ and $\theta_2(x, y)$ such that

$$\theta_1(x, y) = k_1 x + k_2 y, \qquad \theta_2(x, y) = k_1 x - k_2 y,$$
$$k_1 = \cos(\alpha), \ k_2 = \sin(\alpha),$$

and are parametrized by the angle α.

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- M. Haragus & A. Scheel, *Grain boundaries in the Swift-Hohenberg equation*, European J. Appl. Math. **23**, 737-759 (2012).

- A. Scheel & Q. Wu, *Small-amplitude grain boundaries of arbitrary angle in the Swift-Hohenberg equation*, Z. Angew. Math. Mech. **94**, 203-232 (2014).

- D.J.B. Lloyd & A. Scheel, *Continuation and Bifurcation of Grain Boundaries in the Swift-Hohenberg Equation*, SIAM J. Appl. Dyn. Sys. **16**, 252-293 (2017).

The regularized Cross-Newell equation

$$\tau(k^2)\frac{\partial\theta}{\partial t} = -\nabla\cdot\left(\vec{k}B(k^2) + \Delta\vec{k}\right), \qquad \vec{k} = \nabla\theta \qquad \text{(RCN)}$$

Formally derived from SH by means of a multiple scales expansion, assuming $\psi(x,y) \simeq \psi_0(\Theta/\epsilon)$ and

$$\Theta = \epsilon\theta, \quad X = \epsilon x, \quad Y = \epsilon y, \quad T = \epsilon^2 t, \quad \epsilon << 1.$$

For k^2 near 1, $\tau(k^2) \simeq 1$, $B(k^2) \simeq 2(1-k^2)$, and RCN becomes

$$\begin{aligned} \frac{\partial\theta}{\partial t} &= -\nabla\cdot\left(2\vec{k}(1-k^2) + \Delta\vec{k}\right), \qquad \vec{k} = \nabla\theta \\ &= -\frac{1}{2}\frac{\delta\mathcal{E}_{RCN}}{\delta\theta}, \qquad \mathcal{E}_{RCN} = \int_\Omega \left[(\Delta\theta)^2 + (1-|\nabla\theta|^2)^2\right] d\Omega \end{aligned}$$

- M.C. Cross & A.C. Newell, *Convection patterns large aspect ratio systems*, Physica **D 10**, 299-328 (1984).
- N.M. Ercolani, R. Indik, A.C. Newell & T. Passot, *The Geometry of the Phase Diffusion Equation*, J. Nonlinear Sci. **10**, 223-274 (2000).

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Knee solutions of the regularized Cross-Newell equation

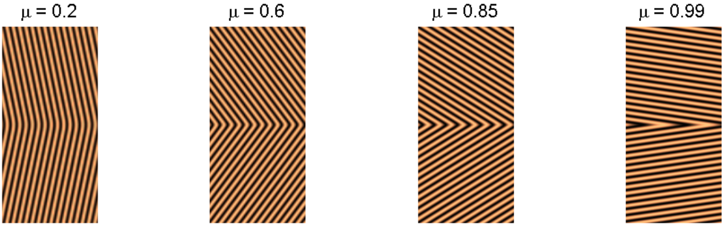
The regularized Cross-Newell equation

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \left(2\vec{k}(1-k^2) + \Delta \vec{k}\right), \qquad \vec{k} = \nabla\theta$$

admits exact solutions

$$\theta(x,y) = \sqrt{1-\mu^2}\, x - \log\left(2\cosh(\mu y)\right)$$

that correspond to grain boundaries when looking at level sets of the phase θ, or for instance at $\cos(\theta)$.



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Knee solutions of the regularized Cross-Newell equation

- Knee solutions of RCN are minimizers of the RCN energy $\mathcal{E}_{RCN}$ in the space $\mathcal{F}$ of functions $\theta(x, y)$ such that
  - $\theta \in H^2(\Omega)$, $\Omega = [0, P] \times [-L, L]$, $P = \pi/\sqrt{1-\mu^2}$;
  - $\theta(x+P, y) = \theta(x, y), \qquad \forall y \in [-L, L]$;
  - $\theta_x = \sqrt{1-\mu^2}, \quad \theta_y = \pm\mu \tanh(\mu L), \quad$ at $y = \pm L$,

  that is for functions whose gradients are vector fields.

- In agreement with the above nonlinear result, the second variation of $\mathcal{E}_{RCN}$ is positive for all modal perturbations that satisfy the boundary conditions.

Joint work with N. Ercolani and N. Kamburov

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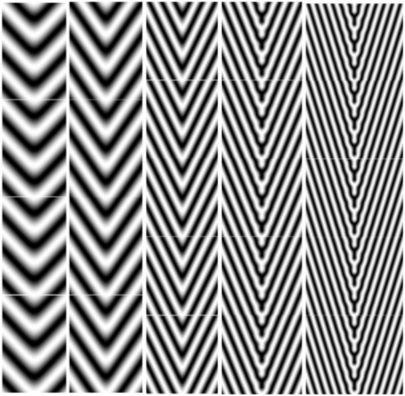
Grain boundaries of the regularized Cross-Newell equation

Numerical minimizers of the RCN energy with mixed Dirichlet-Neumann boundary conditions along the core of the grain boundary also show the existence of a symmetry-breaking bifurcation.

Right: Numerical solutions of the RCN equation.

0.25π 0.3π 0.35π 0.37π 0.4π



N.M. Ercolani & S.C. Venkataramani, *A Variational Theory for Point Defects in Patterns*, J. Nonlinear Sci. **19**, 267-300 (2009).

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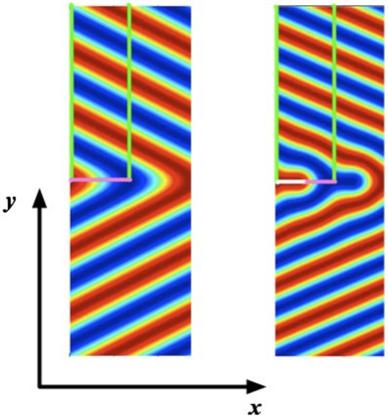
Mixed Dirichlet-Neumann boundary conditions



Solutions are such that

$$\theta(x,0) = 0 \quad \text{for } 0 \le x \le al,$$

$$\theta_y(x,0) = 0 \quad \text{for } al \le x < l,$$

where $\theta(x,y) - k_1 x$ is periodic in x with period l for each $y \ge 0$, and $0 \le a \le 1$.

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N.M. Ercolani & S.C. Venkataramani, *A Variational Theory for Point Defects in Patterns*, J. Nonlinear Sci. **19**, 267-300 (2009).

- Consider the following vector function of $\vec{k} = (f, g)$

$$\vec{S}(\vec{k}) = 2\left(\int (1-k^2)\, df, -\int (1-k^2)\, dg\right).$$

- Show that for $\vec{k} = \nabla\theta$, i.e. $f = \theta_x$, $g = \theta_y$, $\theta_{xy} = \theta_{yx}$,

$$\int_\Omega \left(-\nabla \cdot \vec{S}(\nabla\theta) + 4\,\mathrm{det}(\mathrm{Hess}(\theta))\right) d\Omega \leq \mathcal{E}_{RCN}(\theta).$$

- Note that the left-hand side of the above only depends on the boundary conditions satisfied by functions in $\mathcal{F}$ and conclude that all $\theta \in \mathcal{F}$ (such that $\nabla\theta$ is globally defined as a vector field on Ω) satisfy

$$\mathcal{M} \equiv 4P\mu^3\left(\tanh(\mu L) - \frac{1}{3}\tanh^3(\mu L)\right) \leq \mathcal{E}_{RCN}(\theta).$$

- Evaluate $\mathcal{E}_{RCN}$ on the knee solution θ_0 and note that $\mathcal{E}_{RCN}(\theta_0) = \mathcal{M}$.

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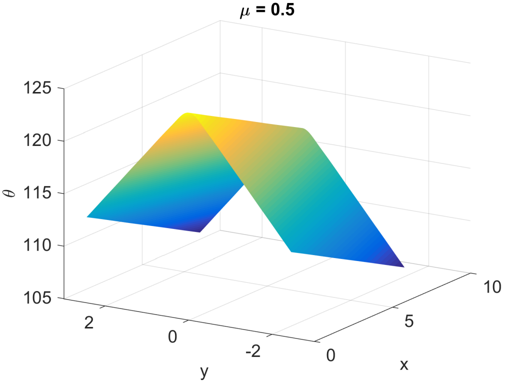
Phase gradient of SH Grain boundaries - small μ's

For small values of μ the phase behaves like a "knee" solution.

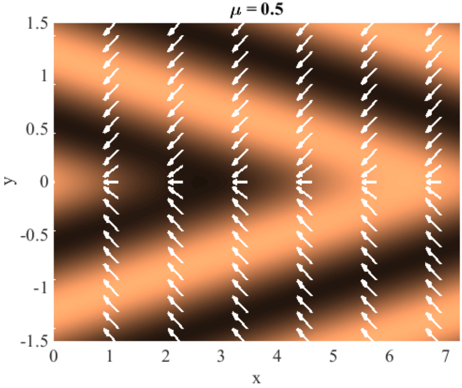
Right: Phase as a function of x and y



Phase gradient of SH Grain boundaries - small μ's

For small values of μ the phase behaves like a "knee" solution.

Right: Phase gradient superimposed on grain boundary



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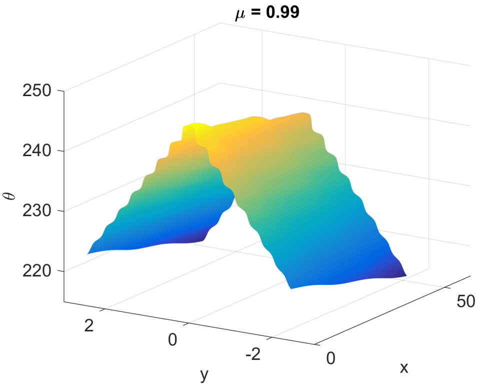
For large values of μ the y-derivative of the phase gets very large on each sides of the grain boudary.

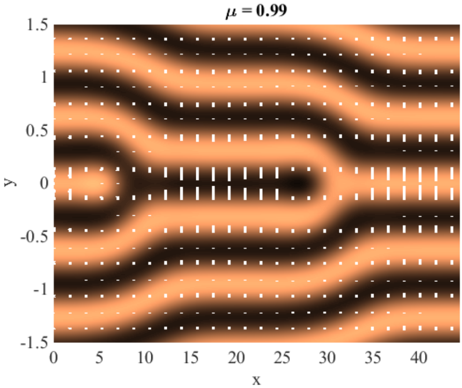
Right: Phase as a function of x and y



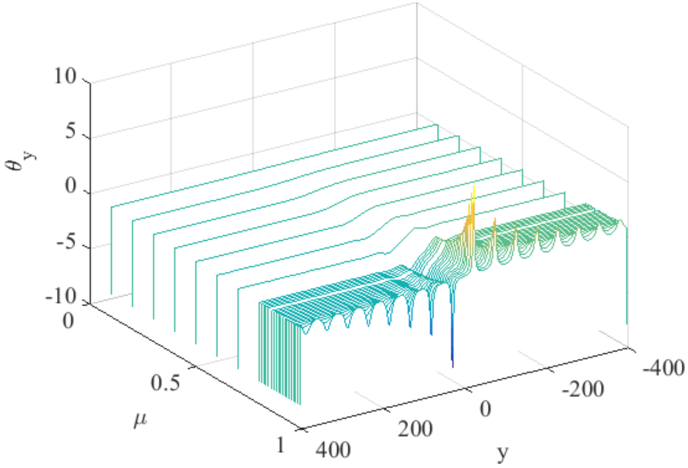
Phase gradient of SH Grain boundaries - large μ's

For large values of μ the y-derivative of the phase gets very large on each sides of the grain boudary.

Right: Phase gradient superimposed on grain boundary



Phase structure of SH Grain boundaries - jump in θ_y



Profile of θ_y at $x = L_x/2$ as a function of y, for different values of μ.
The grain boundary is located at $y = 0$.

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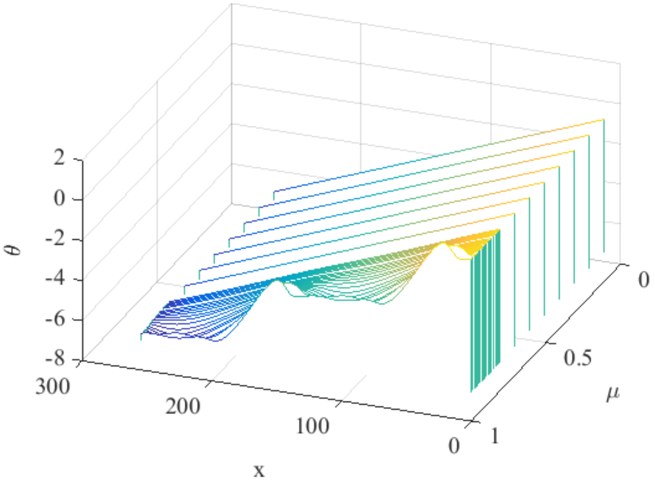
Phase structure of SH Grain boundaries



Profile of θ on one side of the "jump" as a function of x, for different values of μ.

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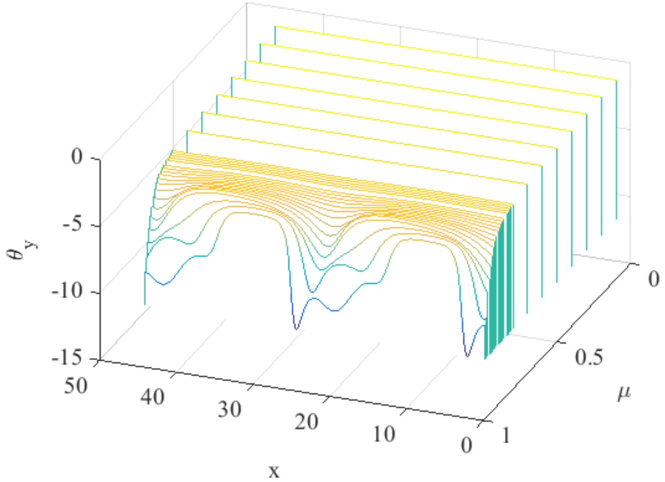
Phase structure of SH Grain boundaries



Profile of θ_y on one side of the "jump" as a function of x, for different values of μ.

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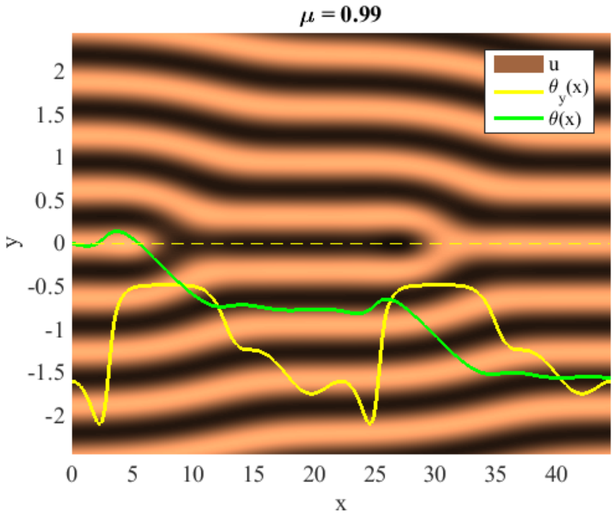
Phase structure of SH Grain boundaries



Profile of θ and θ_y on one side of the "jump" as a function of x superimposed on the grain boundary solution.

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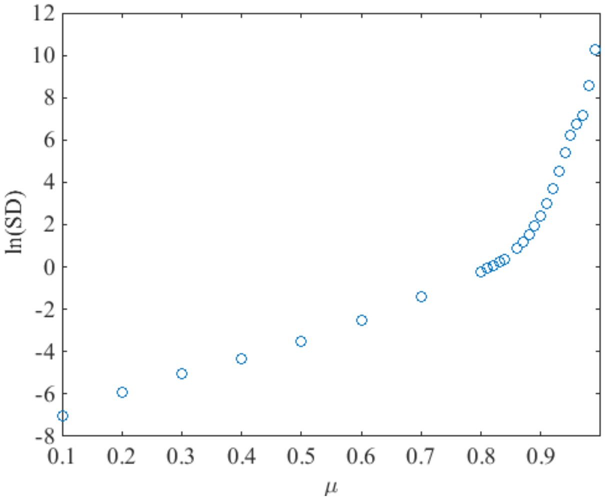
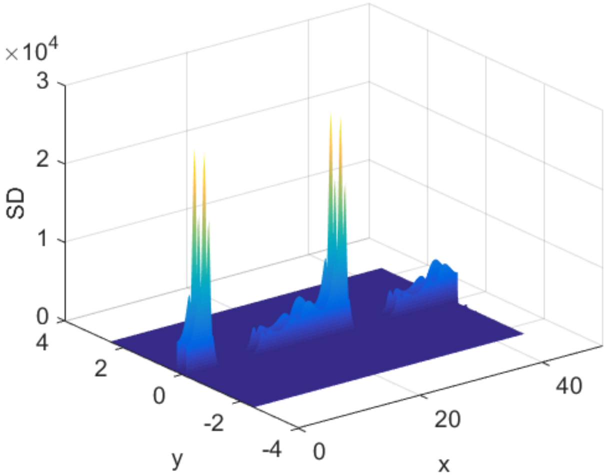
Phase structure of SH Grain boundaries - self-duality



Deviation from self-duality of the phase of SH grain boundaries:
$SD = ||(\Delta\theta)^2 - (1 - |\nabla\theta|^2)^2||_\infty$.

Phase structure of SH Grain boundaries - self-duality



Deviation from self-duality of the phase of SH grain boundaries:
$SD = |(\Delta\theta)^2 - (1 - |\nabla\theta|^2)^2|$.

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